Conformation dependent electronic transport in a DNA double-helix

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In this work we report the study of conformation dependent electronic transport properties of DNA double-helix within tight-binding framework including its helical symmetry. We have studied the changes in localization properties of DNA as we alter the number of stacked bases within a pitch of the double-helix keeping the total number of nucleotides in the DNA chain fixed. We take three DNA sequences, two of them are periodic and one is random and observe that localization length increases as we increase the radius of DNA double-helix *i.e.*, number of nucleotides within a pitch. We have also investigated the effect of backbone energetic on the I-V response of the system and we find that in presence of helical symmetry, depending on the interplay of conformal variation and disorder strength DNA can be found in either metallic or semiconducting and even in an insulating phase, which in turn successfully explain all the experimental findings by a single model.

I. INTRODUCTION

The advancements of nanoscience and technology with everyday encouraging a growing number of scientists across the various disciplines to devise ingenious ways for decreasing the size and increasing the performance of the nano-electronic circuits. One of the promising route is to use molecules and molecular structures as a component of those circuits. From these efforts a new branch has emerged called molecular electronics. Among different branches of molecular electronics, DNA and alike biomolecules have drawn maximum attention in the last decade from both the theoreticians as well as experimentalists and still growing in numbers. The main reason behind this attraction is the potential of DNA to become an inevitable agent for the future nanoelectronic devices and computers, as it might can serve in different ways in a nano-electronic circuits such as a wire, transistor or a switch depending on its electronic properties [1, 2]. Not only this, a precise knowledge of charge transfer mechanism through DNA could help in understanding the process like oxidative damage sensing, protein binding, gene regulation and cell division. On the other hand electrical properties, specially conductivity of DNA can be used for marker-free gene test [3] which is one of the most highly desired biophysical methods [4]. Inspite of the vast efforts from physicists as well as biologists around the world, charge transport results through DNA are still quite controversial [5–11]. Experimentally it is found that DNA can behave either as a good conductor [5], semiconductor [6, 11], insulator [10, 12] and even as a superconductor [13] at low temperature. Several experiments both on synthetic periodic DNA chains [6, 11] as well as unordered sequence of basepairs [14, 15] show the presence of a conduction gap in I-V curves at room temperature. Whereas linear response observed in Ref. [16] and both

the staircase and linear behaviour in I-V curves shown in poly(dG)-poly(dC) chains [17]. Due to this experimental ambiguity and lack of understanding of charge transfer mechanism in DNA, leads to different phenomenological models in which charge transfer is mediated via polarons [18], solitons [19] or electrons or holes [2, 20, 21].

This diversity of experimental findings on transport properties of DNA is due to several reasons such as, DNA varies widely in terms of its composition, length and structure, presence of counterions and impurities which can attach to the phosphate group of the backbones, environmental effects, thermal vibration and contact resistance variation. In this communication, we try to address the effects of structure of DNA *i.e.*, conformal behaviour on its transport properties. Experiments done more than half a century ago by Wilkins *et. al.*, [22] first suggested that overstretched DNA (quite longer than its natural length) undergoes transition to a structure that can accommodate elongation up to twice the length of a relaxed DNA. Crucial developments in understanding mechanical properties of DNA was achieved via stretching experiments [23–25]. Depending on the stretching force applied, DNA first uncoils, then exhibit stiff elastic response and at last undergoes an abrupt structural transformation. Now as all the DNA are twisted (natural double-helix structure) and the amount of twist-stretch *i.e.*, radius of the helix varies from one situation to another, this study has to be made in details. People have already tried to study the effects of conformation introducing twist angle or chirality [26, 27] into *ab-initio* calculations. Studies also have been done on electronic properties of stretched DNA [28] but the effects of helical structure and conformality on its transport properties are yet not well explored. While study within much simpler tight-binding framework is hardly available in current literature. In our work we try to find out these effects within the tight-binding model. To do this we follow Ref. [29], where a mechanical model of DNA is proposed. DNA being modelled as an elastic rod, wrapped helically by a stiff wire. The radius of elastic rod can change upon stretching with a Poisson's ratio $\eta=0.5$. The outer wire is

affixed to the rod helically with a given pitch. As stretching force being applied, the elastic rod elongates in the length and its radius decreases. As a result the stiff wire overwinds and the number of turn increases. We take this mechanical model and interpret in the language of tight-binding formulation. We use twisted ladder model [30], to imitate this mechanical model which includes both the helical symmetry and conformation. We have been able to show three different phases of DNA *i.e.*, metallic, semiconducting and insulating depending on helical symmetry, conformation (twist-stretching) and disorder. We have also found some structural configurations at which system hardly disturbed by external changes.

This paper is organized in the following way: In Sec. II we discuss about our theoretical formulation and describe the model Hamiltonian. We explain our numerical results in Sec. III and summarized in Sec. IV.

II. MODEL AND THEORETICAL FORMULATION

DNA, carrier of genetic code of all forms of life, a π-stacked array of four different nitrogenous bases adenine (A), guanine (G), cytosine (C) and thymine (T) attached among themselves via hydrogen bond following complementary base pairing and coupled with sugar-phosphate backbones forming the double-helix structure. In most of the theoretical models, electronic conduction [31–35] is assumed through the long-axis of the DNA molecule. To model DNA, in our present study, we take the tight-binding (TB) dangling backbone ladder model [36, 37] and add extra hopping channels due to the proximity of bases in the upper strand with the corresponding bases of the lower strand in the next pitch to incorporate its helical symmetry. The Hamiltonian for the said model can be expressed as (for schematic representation of this model we refer to [30])

$$H_{DNA} = H_{ladder} + H_{helicity} + H_{backbone} , \qquad (1)$$

where,

$$H_{ladder} = \sum_{i=1}^{N} \sum_{j=I,II} \left(\epsilon_{ij} c_{ij}^{\dagger} c_{ij} + t_{ij} c_{ij}^{\dagger} c_{i+1j} + \text{H.c.} \right)$$
$$+ \sum_{i=1}^{N} v \left(c_{iI}^{\dagger} c_{iII} + \text{H.c.} \right) , \quad (2)$$

$$H_{helicity} = \sum_{i=1}^{N} v' \left(c_{iII}^{\dagger} c_{i+nI} + \text{H.c.} \right) , \qquad (3)$$

$$H_{backbone} = \sum_{i=1}^{N} \sum_{j=I,II} \left(\epsilon_i^{q(j)} c_{iq(j)}^{\dagger} c_{iq(j)} \right.$$
$$\left. + t_i^{q(j)} c_{ij}^{\dagger} c_{iq(j)} + \text{H.c.} \right) , \quad (4)$$

where $c_{ij}^{\dagger}$ and c_{ij} are the electron creation and annihilation operators at the ith nucleotide at the jth stand, t_{ij} = nearest neighbour hopping amplitude between nucleotides along the jth branch of the ladder, ϵ_{ij} = on-site energy of the nucleotides, $\epsilon_i^{q(j)}$ = on-site energy of the backbone site adjacent to ith nucleotide of the jth strand with $q(j) =\uparrow,\downarrow$ representing the upper and lower strands respectively, $t_i^{q(j)}$ = hopping amplitude between a nucleotide and the corresponding backbone site, v = interstrand hopping integral between nucleotides in two strands of ladder within a given pitch, v' = interstrand hopping integral between neighboring atomic sites in the adjacent pitches which actually accounts for the helical structure of DNA. Here n denotes the number of sites in each strand within a given pitch. For simplicity, we set $\epsilon_i^{q(j)} = \epsilon_b$, $t_{ij} = t_i$ and $t_i^{q(j)} = t_b$.

To explore the transport properties of DNA, we use semi-infinite 1D chains as source (S) and drain (D) electrodes connected to alternative strands of the DNA in cross-wise fashion to the left and right ends respectively and the Hamiltonian of the entire system is given by $H = H_{DNA} + H_S + H_D + H_{tun}$. The explicit form of H_S, H_D and H_{tun} are

$$H_S = \sum_{i=-\infty}^{0} \left(\epsilon c_i^{\dagger} c_i + t c_{i+1}^{\dagger} c_i + \text{H.c.} \right) , \qquad (5)$$

$$H_D = \sum_{i=N+1}^{\infty} \left(\epsilon c_i^{\dagger} c_i + t c_{i+1}^{\dagger} c_i + \text{H.c.} \right) , \qquad (6)$$

$$H_{tun} = \tau \left(c_0^{\dagger} c_1 + c_N^{\dagger} c_{N+1} + \text{H.c.} \right) , \qquad (7)$$

where τ is the tunneling matrix element between DNA and the electrodes.

To obtain transmission probability $T(E)$ of electrons [38, 39] through DNA double-helix for this two-probe set up, we use the Green's function formalism. The single particle retarded Green's function operator representing the complete system *i.e.*, ds-DNA and two semi-infinite electrodes, at an energy E can be written as $G^r = (E - H + i\eta)^{-1}$, where $\eta \to 0^+$ and H is the Hamiltonian of the entire system. Using Fisher-Lee [38–40] relation the two terminal transmission probability is defined as $T(E) = \text{Tr}[\Gamma_L G^r \Gamma_R G^a]$, where E being the incident electron energy and the trace is over the reduced Hilbert space spanned by the DNA molecule. The effective Green's functions can be expressed in the reduced Hilbert space in terms of the self-energies of the source and drain electrodes $G^r = [G^a]^{\dagger} = [E - H_{DNA} - \Sigma_S^r - \Sigma_D^r + i\eta]^{-1}$, where $\Sigma_{S(D)}^{r(a)} = H_{tun}^{\dagger} G_{S(D)}^{r(a)} H_{tun}$ and $\Gamma_{S(D)} = i[\Sigma_{S(D)}^r - \Sigma_{S(D)}^a]$, $G_{S(D)}^{r(a)}$ being the retarded (advanced) Green's function for the source (drain) electrodes. Here $\Sigma_{S(D)}^r$ and $\Sigma_{S(D)}^a$ are the retarded and advanced self-energies of the source (drain) electrodes due to its coupling with the DNA molecule. It can easily be shown that the coupling matrices $\Gamma_{S(D)}$ corresponding to the couplings of the DNA chain to the source (drain) elec-
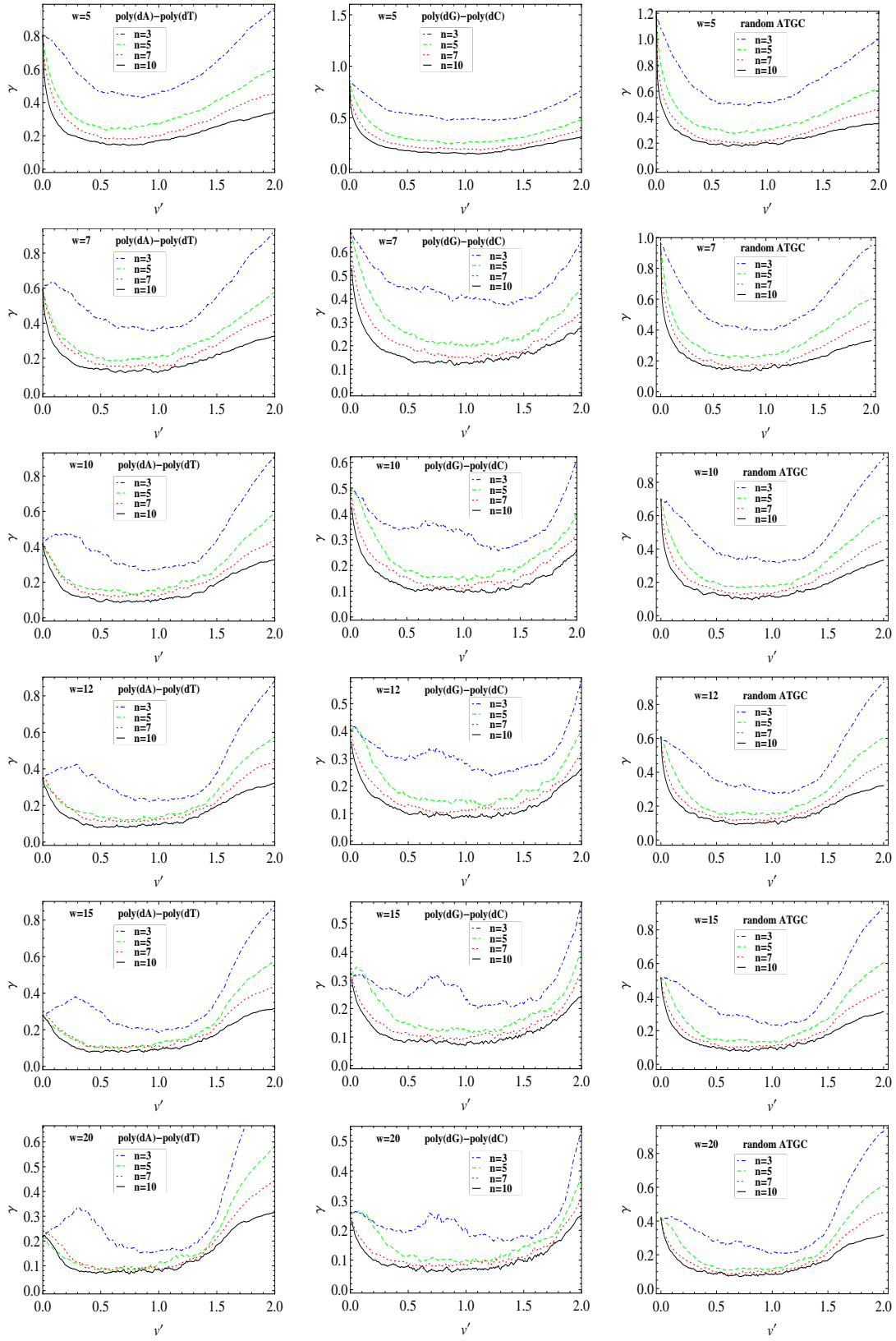
FIG. 1: (Color online). Lyapunov exponent (γ) vs v' for three DNA sequences at several disorder strengths (w), for four different values of n = 3, 5, 7, 10. γ decreses with increasing values of n for all the sequences irrespective of disorder strength, though the features of localization curves are claerly distinguishable for different sequences. There is no distinct changes for the critical values of v' (say, v'_c) which corresponds to the minima of γ with n.

trodes $\Gamma_{S(D)} = -2 \, \text{Im}(\Sigma^r_{S(D)})$. Whereas the self-energies are the sum of $\Sigma^r_{S(D)} = \Delta_{S(D)} + i\Lambda_{S(D)}$, $\Delta_{S(D)}$ being the real part of $\Sigma^r_{S(D)}$ corresponds to the shift of energy levels of DNA, and the imaginary part $\Lambda_{S(D)}$ is liable for the broadening of these levels.

Considering linear transport regime, at absolute zero temperature, the two terminal Landauer conductance is given by $g = \frac{2e^2}{h} T(E_F)$, and the current passing through the DNA chain for an applied bias voltage V can be written as

$$I(V) = \frac{2e}{h} \int_{E_F - eV/2}^{E_F + eV/2} T(E) dE , \qquad (8)$$

where E_F being the Fermi energy. Here we have assumed that entire voltage drop occurs only at the boundaries of the conductor.
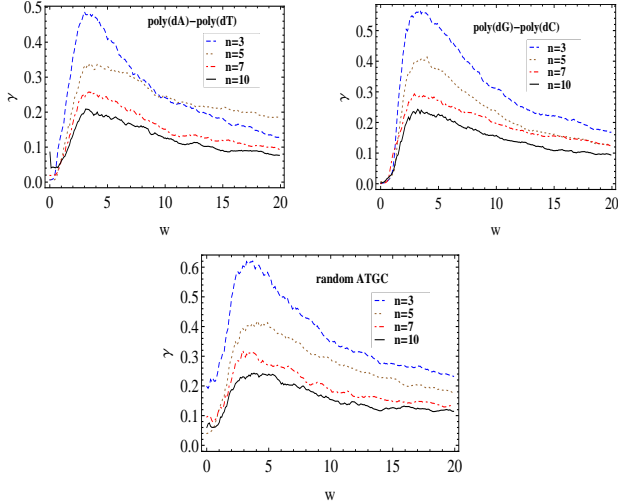
III. RESULTS AND DISCUSSIONS

FIG. 2: (Color online). Lyapunov exponent (γ) vs disorder (w) for three DNA sequences with v'=0.3 eV, for four different values of n = 3, 5, 7, 10. Unifrom behaviour of localization has been observed for all the sequences for whole range of disorder.

We first study the localization properties of the system by altering the number of bases in a given pitch of the helical structure. In order to do that we define localization length (l) from Lyapunov exponent (γ) [41],

$$\gamma = 1/l = -\lim_{L \to \infty} \frac{1}{L} < \ln(T(E)) > , \qquad (9)$$

where L = length of the entire DNA chain in terms of basepairs, and $<>$ denotes average over different disorder configurations. Though other distribution functions e.g., Gaussian and binary have been used to simulate experimental effects in previous studies [36], but we
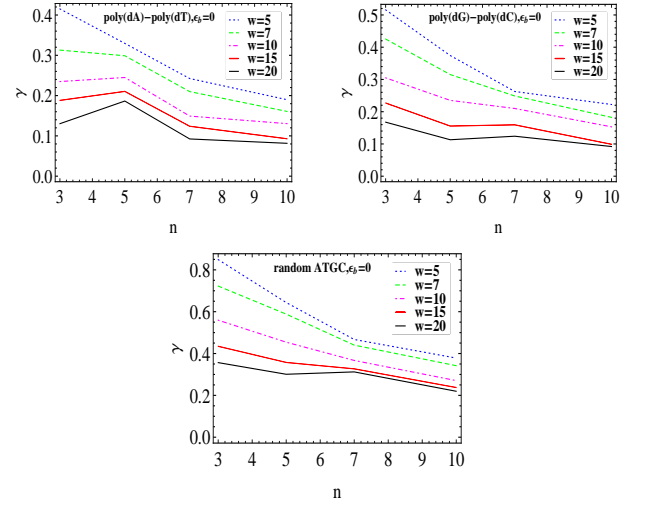

FIG. 3: (Color online). Lyapunov exponent (γ) vs number of nucleotides within a pitch (n) for three DNA sequences with v'=0.3 eV, at different disorder strengths (w). Variation is quite uniform except for poly(dA)-poly(dT) sequence, a sharp peak is present there around n = 5 for heigher values of disorder, showing this may be the most localized configuration for that sequence.

think it is appropriate to employ the most disordered case to simulate the actual experimental complications where the on-site energies of backbones ϵ_b to be randomly distributed within the range $[\bar{\epsilon}_b - w/2, \bar{\epsilon}_b + w/2]$, where $\bar{\epsilon}_b$ is the average backbone site energy and w represents the backbone disorder strength. For the purpose of numerical investigation the on-site energies of the nucleotides are chosen as the ionization potentials of the respective bases, i.e., $\epsilon_G = -0.56eV$, $\epsilon_A = -0.07eV$, $\epsilon_C = 0.56eV$, $\epsilon_T = 0.83eV$. The intrastrand hopping integrals between identical nucleotides are taken as $t = 0.35eV$ while those between different nucleotides are taken as $t = 0.17eV$. We take interstrand hopping parameter to be $v = 0.3eV$. We emphasize that in case of the extended ladder model [42, 43], diagonal hopping between different nucleotides are also taken into account. But as in our case no diagonal hopping being considered, we compensate this by taking a quite larger value of interstrand hopping parameter v. Now as all the nucleotides are connected with sugar-phosphate backbones by identical C-N bonds, we take the hopping parameter between a base and corresponding backbone site same for all $t_b = 0.7eV$ [32]. The parameters used here are the same as those used in [44] which are consistent with *ab initio* calculations [45–47]. For interstrand hopping v' between nucleotides of adjacent pitches we follow Ref [30]. Nevertheless, we want to mention that choice of the tight-binding parameters is not unique and several parameter sets have been proposed in the existing literature [48].

In Fig. 1 we have plotted the variation of inverse localization length (γ) for three sequences with v' (which accounts for the helicity of DNA) at different values of n

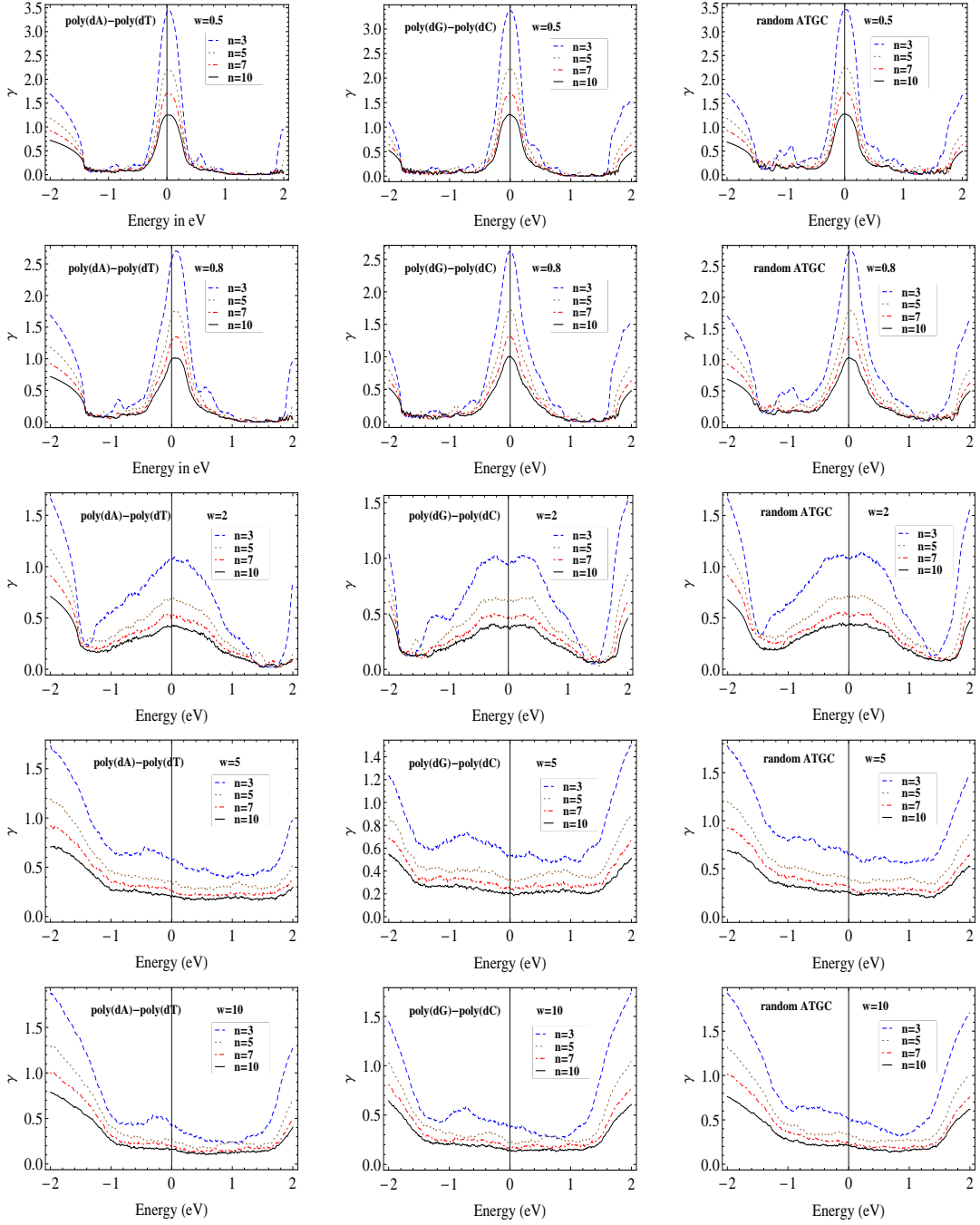FIG. 4: (Color online). Variation of Lyapunov exponent γ with energy (E) for three DNA sequences with v'=0.3 eV, for different values of n. Effect of conformation (n) is stronger at the centre of band for low disorder (w) values, then it shifts towards the band edges for strong disorder.

i.e., number of nitrogen bases within a pitch of the helix, for various values of backbone disorder degree (w). It is clear that all the curves have the same general shape for the periodic as well as the random DNA sequences and the variation of γ with v' is not monotonic. There exists a flat minima in these curves which indicates that at this point system is maximally extended. Now as we vary n (whatever be the disorder strength w is), γ decreases,

which indicates that system is less localized and effects of environmental fluctuations also becoming weaker. This behaviour can be explained easily, as we increase n we are allowing more channels for conduction between two adjacent pitches. As n increases, an electron can eventually hops from one pitch to the next, galloping other nucleotides in that pitch. With increasing n, the length of this gallop also increases *i.e.*, an electron gets the path

to bypass more number nucleotides as it move along the DNA chain. Because of this the effective length become shorter for an electron and it feels less disorder. Hence, first due to helical symmetry system become less localized and then due to conformation (n) it gets more and more extended. So, at this configuration system is hardly effected by external disturbances. This information can help to perform experiments on DNA in more easier way and reproducible results can be generated which is a challenging task for a long time.
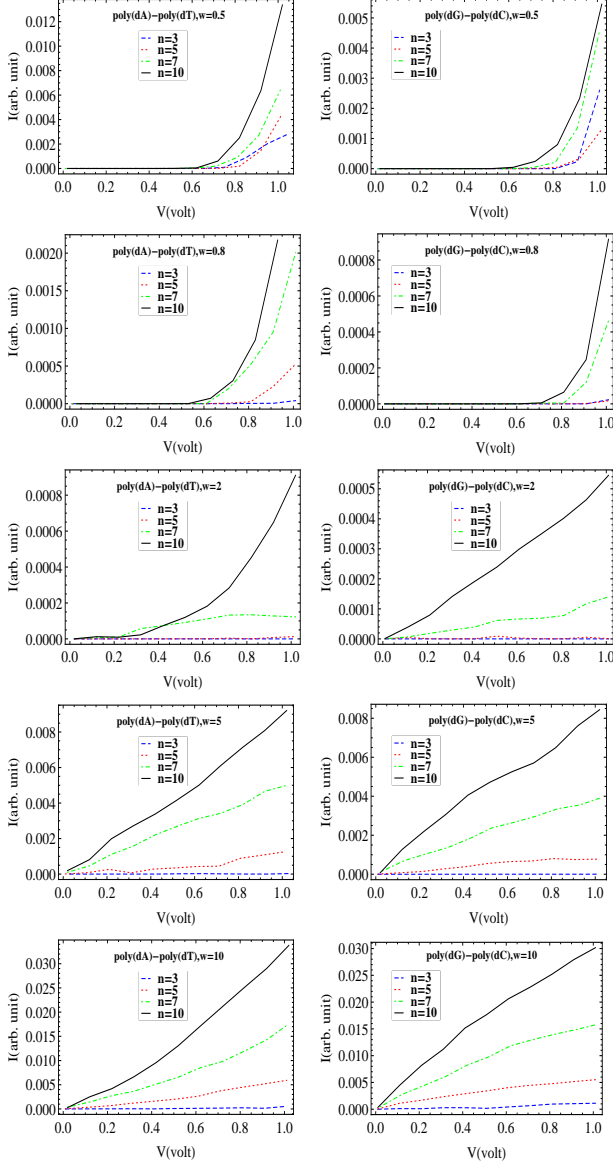

FIG. 5: (Color online). I-V response for two periodic sequences: poly(dA)-poly(dT) and poly(dG)-poly(dC) for five different disorder strength (w) at different values of n. For low disorder, cut off voltage reduces as we increase n, showing semiconducting behaviour. For strong disorder, current is considerably enhanced with increasing n giving a insulator to metallic transition.

In Fig 2 we plot γ vs. disorder strength (w), at a fixed value of v'=0.3 eV, for several values of n. Here also as we increase n, γ decreases for all values of w. But the variation of γ with w is also not unidirectional. γ reaches a peak value for disorder strength within 3<w<4 for all n values being considered. It signifies that at certain disorder level, localization length becomes minimum, which implies that at this point system is most effected by external disturbances. This typical behaviour of localization is due to backbone structure of DNA [44]. The effect of variation of n is also less for low disorder compared to higher ones. The effect of conformation (n) is maximum when the system is at its most localized state (3<w<4).

In Fig 3 we show the variation of γ with n. It also shows with increasing n, γ decreases, except there is some different features around n=5 for one of the sequence (ploy(dA)-poly(dT)). Though the reason is not yet clearly understood but it seems that system may has a critical configuration, at which it does feel environmental effects most as we vary n. Because of that at n=5, γ increases instead of decreasing, showing it is the most localized configuration under appreciable disorder. This behaviour is not present in the other sequences, which shows different localization behaviour depending on sequential variety.

We also investigate localization behaviour with energy. In Fig 4 we plot the variation of γ with energy for different values of n. The same thing is also happened here, with increasing n, γ decreases. Though the rate of decreasing is fast for small n (n=3, 5), then the variation of n become less effective for changes at higher values of n (n=7, 10). Effect is more prominent near centre of the bands for low disorder. As the disorder increases, effect of variation of n gradually delocalize towards the edges. At high disorder, variation is more sensitive around the edges of the band rather being at the centre.

In Fig. 5 we plot I-V characteristics for the two periodic sequences for several values of n. We set the temperature at 0 K. To minimize the contact effects we choose tunnelling parameter τ to be optimum i.e., $\tau=\sqrt{t_{ij} \times t}$ between ds-DNA and the electrodes, where t is the hopping parameter for the electrodes [49]. It is clear that effect of n is less at low disorder which is obvious because at low disorder any path of charge conduction is equivalent as an electron feels almost no potential variation. As the disorder increases effect of n becomes more distinctive. For strong disorder there is substantial variation of potential at different sites and change in n gives an electron more number of shortcut pathways to move along the DNA chain. So, with increasing n, current is enhanced and the effect is sharp for high disorder values. For low disorder values cut-off voltage being reduced with increasing n, showing semiconductor-like transport. At high disorder for both the periodic sequences, current is considerably enhanced and almost linear response is observed at higher values of n, which indicates a transition from insulating to metallic phase. Our results are consistent with several experimental findings [5, 6, 10].

IV. CONCLUDING REMARKS

Till now different models have been used to study transport properties of DNA but none of these has taken into account of helical symmetry which is a basic feature of DNA structure. Using twisted ladder model we first incorporate the helicity and then by varying the number of nucleotides within a pitch we try to model the conformational variation of DNA. Though some calculations are present in the literature [26–28] but investigation within tight-binding framework is lacking. We report that depending on helical symmetry and conformation, localization properties can change considerably. The effect of conformation is less when environmental complications are small and increases with it. We have two interesting results. First one is by incorporating helical symmetry and conformation we have been able to minimize the environmental effects to a great extent. It is clear from localization data that interplay of helical symmetry and conformation can provide some configurations where system is hardly disturbed by external agencies.

If this information can be used correctly in experiments, we think the operation of such experiments would become less complicated. We investigated these properties in every aspect possible and it shows unambiguous variation with conformational changes. The second result is, in presence of helical symmetry, depending on the cooperative effect of backbone disorder and conformation system can undergo a transition from insulating to metallic phase as it is eminent from the I-V responses of periodic sequences for higher disorder values. Whereas for low disorder with increasing n, cut-off voltage being reduced for semiconducting response. In summary, we can say that conformal changes have prominent effects on charge transport properties of DNA as it shows that DNA can be found in three different phases e.g., insulating, semiconducting and metallic depending on the mutual variation of environmental fluctuations and conformation. We hope in near future our results will be tested experimentally to find exact effects of helical symmetry as well as conformation on transport properties of DNA.

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